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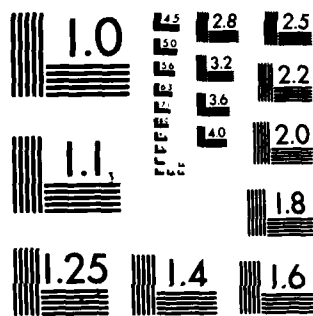
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WATER QUALITY OPTIMIZATION THROUGH SELECTIVE WITHDRAWAL

By Aubrey B. Poore and Bruce Loftis

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operation strategy, and a linear constraint set. These constraints include the hydraulic characteristics of the outlet works and any specified bounds on the release concentrations of the water quality parameters. Two different problem formulations are addressed. The target-concentration problem is formulated to achieve specific downstream target concentrations without actual constraints on the release concentrations. The constrained-concentration problem is formulated to allow the specification of upper and lower bounds for all or some of the water quality constituents. Both formulations can accurately deal with the hydraulic complexity of a multilevel outlet works.

The algorithms presented herein can be used to regulate a reservoir in a real-time mode in which the state of the system is known by actual measurements. The algorithms can also be used with an ecosystem simulation model in which the state of the system is predicted.

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PREFACE

The analysis and technique development reported herein were conducted under Task IID.2, Reservoir Regulation Techniques for Water Quality Management, of the Environmental and Water Quality Operational Studies (EWQOS). The analysis and development were conducted during the period May 1978-August 1980 in the Hydraulics Laboratory of the U. S. Army Engineer Waterways Experiment Station (WES) under the general direction of Mr. H. B. Simmons, Chief of the Hydraulics Laboratory, Mr. John L. Grace, Jr., Chief of the Hydraulics Structures Division, and Dr. Dennis R. Smith, Chief of the Reservoir Water Quality Branch. The analysis and development were conducted and the report prepared by Dr. Aubrey B. Poore and Mr. Bruce Loftis. Dr. Jerome L. Mahloch of the Environmental Laboratory was the Program Manager of EWQOS.

Commander and Director of WES during the preparation and publication of this report was COL Tilford C. Creel, CE. Mr. Fred R. Brown was Technical Director.

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WATER QUALITY OPTIMIZATION THROUGH SELECTIVE WITHDRAWAL

PART I: INTRODUCTION

1. As a result of increasing public awareness and recent State and Federal legislation, water quality considerations in the operation of water resources systems are assuming a significant priority. Multilevel outlet works are the primary method for controlling the quality of releases from stratified lakes. These structures allow the release of water from various vertical strata in the lake. Typically, lakes are operated to enhance the water quality of a downstream fishery or to maintain preproject downstream temperature characteristics, but a wide range of operating strategies can be envisioned to satisfy different water quality needs.

Purpose

2. The purpose of this report is to discuss the problem of operation of a multilevel outlet structure for water quality purposes and to present algorithms for identifying an optimal operating strategy that considers many different water quality constituents.

3. The algorithms presented are for use within a numerical model that simulates the ecosystem of a lake through time but could be applied to operation of a real-time system.

Overview

4. Operation of multipurpose lakes to meet water quality objectives is fundamentally a matter of making trade-offs among such aspects as ports, water quality parameters, time periods, and even project purposes and projects. Further, in a density-stratified lake, concentrations of water quality constituents vary with elevation. Thus, for projects with multilevel intake structures, trade-offs among ports must

be evaluated to determine which ports should be opened and what the flow rate should be through each port in order to meet downstream water quality requirements.

5. Another type of trade-off in lake management exists among water quality parameters. Often, operation to meet goals for several water quality parameters results in conflict, an example of which is downstream water quality requirements for water with both a low temperature and a high dissolved oxygen content to promote a cold-water fishery. In the summer, water in the top of the pool usually has a high temperature and high dissolved oxygen (DO) content, whereas water in the bottom of the pool is normally low in temperature and DO concentrations. A decision must often then be made to either withdraw surface water, thereby fulfilling the DO requirement but failing to meet the temperature requirement, or to withdraw bottom water, thereby achieving the temperature objective but failing to meet the DO objective. A possible trade-off between parameters would be to assign weights to each of them and operate to meet both objectives as closely as possible by mathematically minimizing deviations from the objectives in accordance with the specified weights.

6. A third type of trade-off involves balancing quality in time. It is possible to operate optimally on a day-to-day basis with no anticipation of future conditions. Such operation, which can be referred to as static-optimal, will result in deviations from the objective throughout the simulation period. For example, a lake can be operated static-optimally to meet target temperatures in spring and summer. However, because bottom water is required to achieve the downstream target temperature in early and mid summer, the cold water needed to meet temperature targets in late summer and fall can be depleted and large deviations then occur. However, if future conditions are known or can be estimated, dynamic-optimal rather than static-optimal operation can smooth out the daily deviations to achieve an overall lower level of deviation. The principle behind dynamic-optimal operation is that a large number of small deviations can have a more favorable impact on the ecosystem than a smaller number of larger deviations. Dynamic-optimal operation can

result in release temperatures that are slightly warmer than desired in summer, thereby saving cold water for fall requirements.

7. A fourth type of trade-off requires making decisions relating to total flow released from a lake in order to balance water quality benefits with benefits or demands from other project purposes such as flood control or hydropower production. During a major flood it is apparent that operation of a lake for flood protection has priority. But during normal hydrologic events, it is possible to consider trade-offs between water quality and other project purposes. For example, a peaking power operation could require so large a release flow rate that the withdrawal zone would extend to the bottom; anoxic water could then be released downstream or the bottom sediments could be disturbed. Therefore, reducing the peaking power could improve the release water quality.

8. A final type of trade-off concerns the operation of a system of lakes and connecting streams to achieve water quality requirements at different locations throughout the system.

PART II: LITERATURE REVIEW

9. Simulation models which use optimization methods to identify reservoir operation strategies for satisfying water quality objectives are relatively new tools in the field of water resources systems analysis. They have been used most often for planning and rarely for real-time operation. Optimization methods have been used to determine size and locations of selective withdrawal intakes (Loftis and Fontane 1976) and to develop improved or simpler operation techniques (Patterson et al. 1977, Maynard et al. 1978). Beard and Willey (1970) developed a thermal simulation model that included a heuristic procedure to anticipate future temperature objectives in determining reservoir operation strategies. Kaplan (1974) combined a lake ecosystem simulation model and a nonlinear optimization technique to determine the best operation of a selective withdrawal outlet structure considering constraints of several water quality parameters. A scalar water quality index that commensurated and prioritized several water quality objectives was used as the objective function for this optimization problem. Farber and Labadie (1978) at Colorado State University combined a state-space dynamic programming algorithm with the "WESTEX" Reservoir Heat Budget Model (Loftis 1979). This combination provided a systematic procedure for determining release temperature regulation strategies that anticipated future meteorological and hydrological conditions. Dynamic programming was selected because it could handle sequential decisions and system nonlinearities conveniently. Fontane, Labadie, and Loftis (1982) developed the technique of objective-space dynamic programming which allocated violations of release temperature from downstream target temperature such that an objective function for the entire stratification cycle was minimized. The Hydrologic Engineering Center has developed the model HEC-5Q (1981) to determine operation strategies for a system of lakes and connecting streams considering water quality as one of many project purposes. The solution technique presented in this report is included in the HEC-5Q model.

PART III: A REVIEW OF KAPLAN'S WORK

10. Kaplan (1974) presented one solution to the multiparameter regulation problem. He used a lake ecosystem simulation model (developed by Water Resources Engineers 1969) to determine the water quality state in each of the various layers of a stratified lake. From the system state, Kaplan extracted the states of those layers that contained ports and constructed a state matrix ϕ such that the p^{th} column represented the water quality state at the p^{th} port.

11. As the objective function for the optimization problem, Kaplan used a scalar water quality index which was a function of the release concentrations of the water quality constituents under consideration. Upper and lower bounds on the release concentrations were problem constraints. Kaplan discovered at least two serious difficulties with the optimization problem.

12. The first difficulty was that the number of constraints was at least two or three times the number of independent variables; thus, it was not always possible to satisfy all constraints. Kaplan devised an elaborate scheme involving three sets of constraints--most stringent, stringent, and least stringent--to resolve this problem of feasible and nonfeasible constraints and the various trade-offs. If the most stringent set of constraints could not be satisfied, the stringent set or the least stringent set was tried until the constraints could be met. A penalty was associated with the stringent and least stringent sets. Kaplan worked out a trade-off between maximizing the water quality index and minimizing the penalty associated with various constraint levels and then decided on an appropriate set of port openings.

13. The second difficulty was the reported existence of multiple maxima; thus, to find the optimum set of port openings, all local maxima points had to be found and the corresponding functional values compared. To find as many local maxima as possible, Kaplan used a random number generator to generate starting points in the feasible search region for the optimization code. These multiple maxima were then used in a trade-off analysis of constraint level and the value of the water quality index.

14. The optimization code used by Kaplan to solve the optimization problem was an all-purpose, parameter-free, penalty function code developed at the University of Texas by Staha and Himmelblau (1972). This code, COMET, was developed to handle any set of general algebraic constraints and makes no allowances for a special structure such as linearity. Kaplan reported that the code occasionally terminated due to round-off error and had to be restarted to reach a local maximum. This termination was accompanied by an objective function with a flat surface, which suggests that there may not, in fact, have been multiple maxima.

15. Once the local maxima were found, the optimal flow rate through each port was determined; then the port openings were used for the next simulation period. The water quality index was found for each layer of the lake down to the thermocline; the arithmetic mean of the indices was computed and used as a representative water quality index for the lake (WQI_{LAKE}). The total water quality index was computed as

$$WQI = \frac{w_1 WQI_{RELEASE} + w_2 WQI_{LAKE}}{w_1 + w_2} \quad (1)$$

where w_1 and w_2 are positive weights indicating the relative value of satisfying in-lake water quality requirements and downstream water quality requirements. By comparing the WQI and the number and severity of the violated constraints, Kaplan was able to decide on a set of port openings to manage the water quality of the lake and river.

16. Kaplan noted that Staha and Himmelblau compared the COMET algorithm to three nonlinear programming codes for 25 test problems. The latter investigators found that with analytically supplied derivatives COMET was decidedly more efficient than the other codes, but it was less so for cases where numerical approximations to the derivatives were used. The derivatives for Kaplan's water quality problem were determined numerically, so it is difficult to compare the efficiency of COMET with that for each of the other nonlinear codes tested. Further, the nonlinear constraints can be transformed to linear constraints which are handled far more efficiently by primal methods than penalty function methods.

17. The problem of multiple maxima is always difficult to resolve. The fact that the objective function is reportedly flat suggests that the algorithm COMET stopped due to small changes in the function values, even though the maximizing points were far from the actual solution.

PART IV: PROBLEM FORMULATION

Water Quality Indices

18. Construction of a water quality index is a mathematical approach that aggregates information on one or more water quality parameters to produce a single number which indicates the relative quality of the water under consideration. Such a scalar index is essential for a mathematical optimization solution to the problem of operation of a lake for water quality management. In order to compute a water quality index for water with known concentrations, it is first necessary to compute subindices for each water quality constituent. For a concentration Y_c of a water quality constituent c , there is an associated subindex S_c that measures the quality of the water based only on constituent c . Graphs of subindex value versus concentration for several constituents as suggested by the National Sanitation Foundation (NSF) are reprinted from Kaplan's thesis with permission and are presented in Figure A1; polynomial approximations to the subindex functions are presented in Table A1; both can be found in Appendix A.

19. There are several ways to combine the water quality subindices into a scalar index. The algorithm presented in this report used an additive NSF index

$$WQI = \sum_{c=1}^{N_c} w_c S_c \quad (2)$$

where

WQI = scalar water quality index

c = index for constituents

N_c = total number of water quality constituents

w_c = relative weighting for constituent c

S_c = water quality subindex value for constituent c

The weights are restricted by

$$0 \leq w_c \leq 1 ; \text{ for all } c \quad (3)$$

and

$$\sum_{c=1}^{N_c} w_c = 1 \quad (4)$$

20. Another form of the water quality index is the multiplicative form as presented by the Environmental Protection Agency (Ott 1978).

$$WQI = \prod_{c=1}^{N_c} S_c^{w_c} \quad (5)$$

where the weights w_c satisfy the same restrictions as they do for the additive water quality index. The multiplicative form is more sensitive to a low subindex value for a particular constituent and could therefore have advantages for some applications. It is more difficult to use the multiplicative index for an optimization problem, however, because derivatives of the water quality index for individual concentrations are quite cumbersome.

Objective Function

21. Two different types of multiparameter regulation problems can be considered. The first, called the constrained-concentration problem, allows an acceptable range of release concentrations for each water quality constituent. The second, called the target-concentration problem, is formulated to achieve specific downstream target concentrations without actual constraints on the release concentrations. An objective function must be developed to solve both types of problems. The objective function presented herein for each of these problems is the additive

form of the water quality index; however, the methodology could easily include any other kind of objective function.

22. To determine the value of the objective function for either type of problem it is first necessary to know the state of the system. A system state matrix is defined to contain the concentrations of the various constituents at each port. This concentration matrix ϕ has elements $\phi_{c,p}$ representing the characteristic concentration of the c^{th} constituent at the p^{th} port. If q_p denotes the flow rate out of the p^{th} port, then the release concentration for constituent c can be determined as a flow-weighted average of the concentration at each port.

$$R_c = \frac{\sum_{p=1}^{N_p} q_p \phi_{c,p}}{\sum_{p=1}^{N_p} q_p} \quad (6)$$

where

- c = index for constituents
- R_c = release concentration for constituent c
- p = index for ports
- N_p = number of ports
- q_p = flow rate through port p
- $\phi_{c,p}$ = concentration of constituent c at port p

Equation 6 is not valid if the water quality constituent under consideration is pH. One method of computing the release pH R_c is

$$R_c = -\log_{10} \left(\frac{\sum_{p=1}^{N_p} q_p 10^{-\phi_{c,p}}}{\sum_{p=1}^{N_p} q_p} \right) \quad (7)$$

For the constrained-concentration problem, the reference concentration Y_c from which the water quality subindex for constituent c can be computed is

$$Y_c = R_c \quad (8)$$

For the target-concentration problem,

$$Y_c = R_c - T_c \quad (9)$$

where T_c equals downstream target concentration for constituent c . Equation 9 is used for temperature for either of the problem formulations. The water quality subindices S_c for each constituent are computed as a polynomial function of the reference concentration Y_c .

$$S_c = S_c(Y_c) \quad (10)$$

For the constrained-concentration problem, suggested subindex functions are determined by curve-fitting the NSF functions in Figure A1. Coefficients for these functions are presented in Table A1. For the target-concentration problem, the subindex functions can be specified as parabolic, with the reference concentration at the vertices of the parabolas. Suggested coefficients for the target-concentration subindex polynomials are presented in Table A2.

23. Thus, the subindex functions can be written as follows

$$S_c = \sum_{k=0}^{\eta_c} a_{k,c} Y_c^k ; \quad c = 1, \dots, N_c \quad (11)$$

where

c = index for constituents

S_c = subindex value for constituent c

k = counter for terms in polynomial representation of subindex functions

η_c = highest order term in polynomial representation for constituent c

$a_{k,c}$ = polynomial coefficient for term k and constituent c

Y_c = reference concentration for constituent c

N_c = number of constituents

The objective function to be maximized can be written as

$$WQI = \sum_{c=1}^{N_c} w_c S_c \quad (2 \text{ bis})$$

Constraints

24. Operation of a lake for water quality management is constrained by characteristics of the outlet structure. The hydraulic structure under consideration is illustrated in Figure 1. The significant components of the structure are two selective withdrawal wetwells, each with a number of selective withdrawal ports, and a single floodgate for larger releases independent of the selective withdrawal system. Constraints on the outlet system include minimum and maximum flow rates through each of the ports. A hydraulic constraint known as thermal blockage requires that only one port in each wetwell can be open at any time. Thus, using the floodgate and one port from each wetwell, a maximum of three ports can be open at any one time. The hydraulic constraints can be expressed as follows

$$F_{\min,p} \leq q_p \leq F_{\max,p} ; \quad p = 1, \dots, N_p \quad (12)$$

where

$F_{\min,p}$ = minimum flow rate that can be released through an open port p

p = index for ports

q_p = flow rate released through port p

$F_{\max,p}$ = maximum flow rate that can be released through port p

N_p = total number of ports in outlet system

This relationship applies only to open ports. A flow rate of zero, which indicates a closed port, is also feasible.

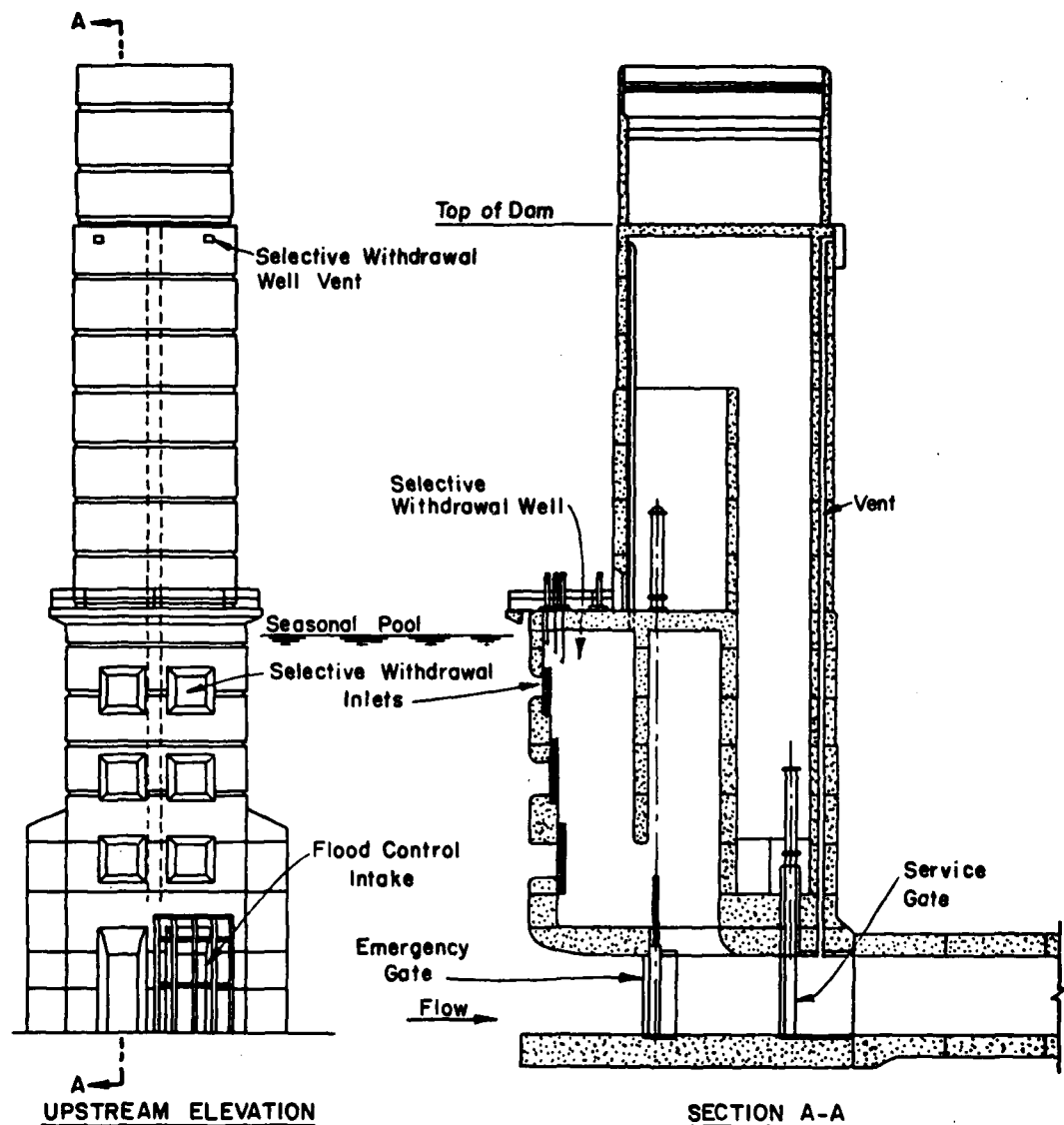


Figure 1. Example selective withdrawal structure

25. The total flow through all of the ports can be constrained to be (a) equal to a specified flow or (b) within a range of flows. Either constraint can be expressed as

$$Q_{\text{lower}} \leq \sum_{p=1}^{N_p} q_p \leq Q_{\text{upper}} \quad (13)$$

where Q_{lower} and Q_{upper} are the minimum and maximum acceptable total flow. If Q_{lower} equals Q_{upper} , then the flow constraint is an equality constraint.

26. The constrained-concentration problem formulation has upper and lower bounds on the release concentrations of each constituent. These concentration constraints take the form

$$Y_{\text{lower},c} \leq Y_c \leq Y_{\text{upper},c} ; \quad c = 1, \dots, N_c \quad (14)$$

where

$Y_{\text{lower},c}$ = lower bound for reference concentration for constituent c

c = index for constituents

Y_c = reference concentration for constituent c

$Y_{\text{upper},c}$ = upper bound for reference concentration for constituent c

N_c = number of constituents under consideration

Formulation

27. The optimization problem can be written to maximize a water quality index subject to hydraulic, flow, and concentration constraints. The concentration constraints are present for the constrained-concentration problem and not present for the target-concentration problem; the decision variables are (a) which ports should be open and (b) what flow rate should pass through each open port. Because there is the hydraulic constraint of only one open port per wetwell, a sequence of optimization problems must be solved. Each of these problems has the following form:

$$\text{Maximize } \sum_{c=1}^{N_c} w_c \left(\sum_{k=0}^{N_k} a_{k,c} Y_c^k \right) \quad (15)$$

subject to

$$F_{\min,p} \leq q_p \leq F_{\max,p} ; \quad p = 1, \dots, N_p \quad (12 \text{ bis})$$

$$Q_{\text{lower}} \leq \sum_{p=1}^{N_p} q_p \leq Q_{\text{upper}} \quad (13 \text{ bis})$$

$$Y_{\text{lower},c} \leq Y_c \leq Y_{\text{upper},c} ; \quad c = 1, \dots, N_c \quad (14 \text{ bis})$$

It should be noted that the last constraint, given in Equation 14, should be deleted for the target-concentration problem.

PART V: SOLUTION PROCEDURE

28. This part describes the solution procedure developed to determine optimum strategy for multiparameter reservoir regulation. It presents (a) the algorithm formulated to address the selective withdrawal system constraints discussed in paragraphs 24-27 and (b) the solution technique for addressing the remainder of the multiparameter constraints.

Selective Withdrawal Outer Loop

29. One of the constraints of the selective withdrawal system is that only one port in each wetwell can be open at any time. This constraint can be expressed mathematically by introducing variables that can only take on the values 0 or 1. Techniques exist for solving problems with 0-1 variables, but only at a large cost in computer resources. Because the problem size is small, then, the most efficient procedure for expressing this constraint is a simple enumeration of alternatives.

30. The algorithm proceeds by considering a sequence of problems, each representing a different combination of open ports. For each combination the optimal allocation of total flow to ports is determined and the value of the objective function is computed for the optimal allocation of flows. The combination of open ports with the largest objective function or water quality index and its associated allocation of flows defines the optimal operation strategy for the time period of interest.

31. There are four different types of combinations of open ports. For one-port problems, all of the flow is taken from a single port and the objective function is computed. For two-port problems, either combinations of one port in each wetwell or combinations of a single port with the floodgate are considered. For three-port problems, combinations of one port in each wetwell and the floodgate are considered. The total flow to be released downstream is specified; if a range of acceptable flows is specified, the flow is treated as an additional decision variable and the flow for which the objective function is maximized is also determined. It should be noted that if the minimum

allowable flow rate through any port $F_{\min,p}$ is zero, then the one-port problem for that port does not have to be included in the enumeration. In fact, if all of the minimum flow rates are zero only the three-port combinations need to be solved.

Overview of Solution Formulation

32. The discussion of the solution techniques and the algorithm for solving the three-port combination flow allocation problem begins by noting that maximizing the water quality index WQI is equivalent to minimizing the negative of WQI, such that $f(q)$ equals $-WQI(q)$. The solution techniques are then more easily explained in terms of the general problem

$$\text{MINIMIZE } f(q) \quad (16)$$

$$\text{SUBJECT TO: } Eq = \underline{e} \quad (17)$$

$$Aq \geq \underline{b} \quad (18)$$

where q is an N_p -dimensional vector representing the flow rates $q = (q_1, \dots, q_{N_p})^T$ and N_p represents the number of ports. E is a matrix of equality constraint coefficients. For this problem there is at most one equality constraint, so E is a row vector and \underline{e} is a scalar. A is a $J \times N_p$ matrix of inequality constraint coefficients, with J representing the number of inequality constraints. The inequality constraint on the right-hand side (\underline{b}) is a J -dimensional column vector. The rows in E are assumed to be linearly independent, while those in A are not. In fact, the number of rows in A can be three to five times larger than the size of q , so that the rows of A are necessarily linearly dependent. Since the objective function $f(q)$ is nonlinear, the problem is a linearly constrained nonlinear programming problem.

33. The field on nonlinear programming is generally decisive in choosing methods for both unconstrained and linearly constrained problems. For linearly constrained nonlinear programming problems, feasible direction methods (Avriel 1976) are generally accepted as the best

optimization techniques. Within this class of techniques the best algorithms are the generalized gradient projection algorithms.

Input Requirements

34. Data requirements for the algorithm include information about the outlet structure, the water quality constituents, and the state of the system. Hydraulic data include the number of ports N_p , the minimum and maximum flow rate through each open port $F_{\min,p}$ and $F_{\max,p}$, the height above the bottom of each port center line H_p , and the wetwell identifier W_p of each port. Selective withdrawal ports are specified to be in wetwell 1 or wetwell 2. The floodgate is defined to be in wetwell 0. Constituent information includes a two-character label for each constituent and the relative weights w_c for adding the subindices in the objective function. For the constrained-concentration problem formulation, the upper and lower acceptable release bounds for each constituent and a target temperature must be specified. For the target-concentration problem formulation, downstream target concentrations must be specified for each constituent. The system state is defined by the depth of the pool, the flow rate Q to be released downstream or the upper and lower bounds Q_{upper} and Q_{lower} on the downstream flow rate, and the concentration matrix ϕ containing the concentration of each constituent at every port.

Initialization of Procedure

35. To initialize the procedure, feasible set of flow rates q^0 must be determined such that the constraints

$$Eq^0 = e \quad (17 \text{ bis})$$

$$Aq^0 \geq b \quad (18 \text{ bis})$$

are satisfied. As an initial estimate, q^0 is taken to be $q^0 = (q_1^0, q_2^0, \dots, q_{N_p}^0)^T$ where

$$q_p^o = \frac{(Q_{\text{lower}} + Q_{\text{upper}})(F_{\text{min},p} + F_{\text{max},p})}{2 \sum_{p=1}^{N_p} (F_{\text{min},p} + F_{\text{max},p})}; \quad p = 1, \dots, N_p \quad (19)$$

This particular choice has worked well in the solution of the problem; however, it does not guarantee that all of the constraints $Aq^o \geq b$ are satisfied. If $Aq^o \geq b$, the iteration procedure begins. Otherwise, a phase-one linear programming procedure can be used to obtain a feasible point when one exists. If no feasible region exists, the q^o defined in Equation 19 is used. The explanation of how particular violated constraints are handled will be given in paragraphs 41-45 on projection matrices. The procedure starts with q^o as defined in Equation 19 because most often $Aq^o > b$. The iteration then begins in the interior of the feasible region and not on the boundary which results from the use of the phase-one linear programming code; thus, movement along the boundary, which slows the convergence drastically, is avoided as often as possible.

General Description of Solution

36. The general scheme of the procedure is to iteratively generate a finite sequence

$$\begin{pmatrix} q^k \end{pmatrix}_{k=0}^{k=N} \quad (20)$$

where q^k is accepted as the optimal set of flows for the given constraints when one of the following is true:

q^k is a Karush-Kuhn-Tucker point

$$\|q^k - q^{k-1}\| < \varepsilon_1 \quad (21)$$

$$|f(q^k) - f(q^{k-1})| < \varepsilon_2 \quad (22)$$

$$k = N \quad (23)$$

where N is some preassigned maximum number of iterations and ε_1 and ε_2 are preassigned small numbers. However, if none of these criteria are satisfied, an updated solution vector of flow rates q^{k+1} is obtained from q^k by choosing a search direction \underline{d}^k and then performing a line search for the minimum in the direction \underline{d}^k from q^k . There are several possible choices for the search direction; e.g., Newton's direction, the negative gradient direction, or the more general variable metric direction (Avriel 1976). Newton's direction at q^k is

$$\underline{d}_{NE} = -H_f^{-1}(q^k) \nabla f(q^k) \quad (24)$$

where the gradient $\nabla f(q)$ is that column vector whose element in the i^{th} position is $\partial f(q)/\partial q_i$ and q_i is the i^{th} element in the vector q . The Hessian matrix of f , $H_f(q)$, is that matrix whose element in the i^{th} row and j^{th} column is $\partial^2 f(q)/\partial q_i \partial q_j$. The negative gradient direction at q_k is

$$\underline{d}_{NG} = -\nabla f(q^k) \quad (25)$$

The procedure presented herein uses a combination of Newton's direction and the negative gradient direction. Assuming that q^k satisfies the constraints, a projection matrix P is constructed to satisfy

$$EP\underline{d}^k = 0 \quad (26)$$

so that

$$E(q^k + \lambda P\underline{d}^k) = \underline{e} \quad (27)$$

$$A(q^k + \lambda P\underline{d}^k) \geq \underline{b} \quad (28)$$

for all λ in some finite range $[0, \lambda_{\max}]$.

37. Initially \underline{d}^k is chosen to be Newton's direction, which is to be preferred near a solution in the interior of the feasible region. If \underline{d}^k and $P\underline{d}^k$ are nonzero descent directions, then the minimum of

$f(q^k + \lambda \underline{P} \underline{d}^k)$ with respect to λ over $[0, \lambda_{\max}]$ is located. The corresponding value of λ at which this minimum occurs is denoted by λ^k , and the next iterate q^{k+1} is defined by

$$q^{k+1} = q^k + \lambda^k \underline{P} \underline{d}^k \quad (29)$$

If Newton's direction or the projected Newton's direction is not a non-zero descent direction, \underline{d}^k is taken to be the negative gradient of f at q^k such that $\underline{d}^k = -\nabla f(q^k)$. In the event \underline{d}^k is zero, q^k is accepted as the optimal flow solution. Otherwise, the projection matrix \underline{P} is again constructed, and $f(q^k + \lambda \underline{P} \underline{d}^k)$ is minimized over $[0, \lambda_{\max}]$ when $\underline{P} \underline{d}^k$ is nonzero. Then q^{k+1} is defined as above in Equation 29. The case

$$\underline{P} \underline{d}^k = \underline{P} [-\nabla f(q^k)] = 0 \quad (30)$$

is special in that q^k may be a Karush-Kuhn-Tucker point and therefore accepted as the optimal solution. (See paragraphs 53-56.) However, if q^k is not a Karush-Kuhn-Tucker point, \underline{P} can be modified so that $\underline{P} \underline{d}^k$ is nonzero and q^{k+1} can be defined as before.

38. The minimization of $f(q^k + \lambda \underline{P} \underline{d}^k)$ over $[0, \lambda_{\max}]$ is called a line search, and Davidon's cubic interpolatory scheme (Walsh 1975) is used in this algorithm. In the sections to follow, these basic ideas are expanded upon and various facets are explained.

Search Directions and Projection Matrices

39. The point q^k is assumed to satisfy the constraints. The unconstrained search direction from the point q^k will be either the negative gradient direction, Newton's direction, or, as mentioned in paragraph 36, one of the variable metric directions (Avriel 1976). Newton's direction \underline{d}_{NE} , as defined in Equation 24, is actually obtained by solving the system of equations

$$H_f(q^k) \underline{d}_{NE} = -\nabla f(q^k) \quad (31)$$

by using Gaussian elimination with scaled partial pivoting.

40. If the point q^k satisfies $Aq^k > \underline{b}$ and there are no equality constraints, then the line search can be performed. However, it is often the case that one of the constraints (i.e., the r^{th} constraint) is active so that $A_r q^k = b_r$, where A_r is the r^{th} row in A . This may be due to the phase-one linear programming technique used to find a starting point q^0 , the existence of solution on the boundary, or the placement of q^k on the boundary for the line search. Now let R be an indexing set defined by

$$R = \{r: A_r q^k = b_r\} \quad (32)$$

so that R enumerates the set of active constraints. If \underline{d}^k is the search direction, it will often happen that $A_r \underline{d}^k$ is negative for some $r \in R$. Then

$$A_r (\underline{q}^k + \lambda \underline{d}^k) < b_r \quad (33)$$

for positive λ , resulting in a violated constraint. The objective then is to construct a projection matrix P , so that $P \underline{d}^k$ is a descent direction producing a negative $\nabla f(q^k) \cdot P \underline{d}^k$. Then $A_r P \underline{d}^k \geq 0$ whenever $A_r q^k = b_r$ and $E P \underline{d}^k = 0$. For λ in some finite interval $[0, \lambda_{\max}]$, the constraints

$$E(\underline{q}^k + \lambda P \underline{d}^k) = \underline{e} \quad (27 \text{ bis})$$

and

$$A(\underline{q}^k + \lambda P \underline{d}^k) \geq \underline{b} \quad (28 \text{ bis})$$

will then be satisfied.

41. The projection matrix used here is constructed as

$$P = I_{N_p} - M^T (M M^T)^{-1} M \quad (34)$$

where I_{N_p} is the $N_p \times N_p$ dimensional identity matrix, M is an $N_m \times N_p$ matrix ($N_m \leq N_p$) whose rows are linearly independent, and M^T denotes the transpose of M . The rows of M are composed of the linearly independent rows of E and, directly or indirectly, those rows of $A(A_r)$ for which $A_r g^k = b_r$. (The explicit algorithm for constructing M is given in paragraph 48.) An important property of the projection matrix P is that $A_r P d = 0$ for any vector d whenever A_r is a row in the matrix M or linearly dependent on rows in M . Other important properties of this projection matrix P are that $PP = P$, $P^T = P$, and $d = Pd + (I_{N_p} - P)d$. Pd is also orthogonal to $(I_{N_p} - P)d$.

42. An optimal choice for P is one that would satisfy

$$A_r P d = 0 \quad \text{if} \quad A_r d \leq 0 \quad (35)$$

and

$$A_r P d \geq 0 \quad \text{if} \quad A_r d \geq 0 \quad (36)$$

That this choice is not always possible can be seen from the relation

$$A_r P d = A_r d - A_r (I_{N_p} - P) d \quad (37)$$

which may be negative because $A_r (I_{N_p} - P) d$ can be larger than $A_r d$.

In his original paper, Rosen (1960) avoided this problem by including in the matrix M , either directly or indirectly, all rows A_r in A for which $A_r g^k = b_r$. Of course, the rows of E must be included in M so that $EP = 0$.

43. The approach taken herein is to begin building the matrix M from the largest linearly independent set of vectors in the collection consisting of all rows in the matrix E and all rows A_r of the matrix A where

$$r \in R = \{r: A_r g^k = b_r\} \quad (38)$$

and

$$A_r \underline{d}^k \leq 0 \quad (39)$$

It may happen that $r \in R$ and $A_r \underline{d}^k > 0$, but $A_r \underline{Pd}^k < 0$. This situation can be avoided by checking the sign of $A_r \underline{Pd}^k$ for each $r \in R$. If $A_r \underline{Pd}^k < 0$ for some r , the row A_r is added to the matrix M and P is updated. This updating procedure is repeated until $A_r \underline{Pd}^k \geq 0$ for all $r \in R$.

44. There are several reasons why this procedure for constructing P should be efficient for this problem. First, it allows the search direction to point into the region from a boundary point. Many optimization procedures lose their efficiency for constrained problems because they artificially require themselves to stay on a boundary until the Karush-Kuhn-Tucker conditions are checked. The small number of independent variables (flow rates) in this problem keeps the updating process from being repeated often. In fact, numerical experimentation indicates that the updating of P rarely occurs more than once, and most often not at all.

45. There are two problems that arise at this point. If \underline{d}^k is Newton's direction, \underline{Pd}^k may not be a descent direction. In this case, \underline{d}^k is redefined to be the negative gradient directions $-\nabla f(\underline{q}^k)$, and P is recalculated for this new \underline{d}^k . If $\underline{d}^k = -\nabla f(\underline{q}^k)$, then \underline{Pd}^k is either zero or a descent direction. That \underline{Pd}^k is a descent direction follows from the identity

$$\begin{aligned} \left[-\nabla f(\underline{q}^k) \right]^T P \left[-\nabla f(\underline{q}^k) \right] &= \left[-\nabla f(\underline{q}^k) \right]^T P^T P \left[-\nabla f(\underline{q}^k) \right] \\ &= \left[-P \nabla f(\underline{q}^k) \right]^T \left[-P \nabla f(\underline{q}^k) \right] \geq 0 \end{aligned} \quad (40)$$

If \underline{Pd}^k is a nonzero descent direction, a line search is performed. Otherwise the Karush-Kuhn-Tucker conditions are checked for the point \underline{q}^k . Either \underline{q}^k is a Karush-Kuhn-Tucker point, or a row in M can be removed and P updated so that $P \left[-\nabla f(\underline{q}^k) \right]$ is a nonzero descent direction.

Violated Constraints

46. At times there are water quality constraints that cannot be satisfied given the constraints on the individual ports and total flow rates. Thus the constraint will be violated at each stage in the iteration. This is handled by including in the indexing set R those rows r for which $A_r \underline{q}^k \leq b_r$. Then $A_r(\underline{q}^k - \lambda P \underline{d}^k) - b_r$ will only increase, with the result that the violated constraint will either improve or stay the same, but will not worsen.

Construction of the Projection Matrix

47. The projection matrix P is constructed in stages from rows in the matrices E and A which arise from the constraints $A \underline{q}^k \geq \underline{b}$ and $E \underline{q} = \underline{e}$. The projection matrix is constructed only in the event there are equality constraints or when the indexing set $R = \{r: A_r \underline{q}^k = b_r\}$ is not empty. The projection matrix P is always defined as

$$P = I_{N_P} - M^T (M M^T)^{-1} M \quad (34 \text{ bis})$$

48. If there are equality constraints, M is initially set by $M = E$ which is an $\ell \times N_P$ matrix with ℓ linearly independent rows. If there are no equality constraints, M is initially defined to be $M = A_r$, a row vector, where r is any index in R for which A_r is nonzero.

49. Several indexing sets are needed in the construction of P . Suppose the unconstrained search direction \underline{d}^k and projection matrix P are as previously defined. Then let

$$R2 = \{r \in R: A_r P \underline{d}^k \leq 0\}$$

$$RL = \{r \in R2: A_r \text{ is linearly dependent on rows in } M\}$$

$$R3 = \{r \in R: A_r P \underline{d}^k > 0\}$$

50. During the construction of P , the indexing sets $R2$, RL , and $R3$ change; however, R does not. The first change in P is made according to the following algorithm. Let P be given by Equation 34 where M is either A_r or E . For each $r \in R2$, proceed according to the following steps:

- a. Calculate $A_r P$.
- b. If $A_r P = 0$, add r to RL .
- c. If $A_r P \neq 0$, add A_r to M , r to RL , and update P .

51. After this algorithm has been completed, the matrix P has generally changed from the original matrix P if R is nonempty. Thus there may be an $r \in R2$ for which $A_r P_d^k > 0$ for the initial P , but for which $A_r P_d^k < 0$ for the final P constructed as in the above algorithm. This problem is rectified in the following manner. Given the projection matrix P from the above algorithm, the following is repeated until $A_r P_d^k > 0$ for each $r \in R3$.

- a. Calculate $A_r P_d^k$ for each $r \in R3$.
- b. If $A_r P_d^k > 0$, leave $r \in R3$.
- c. If $A_r P_d^k \leq 0$, delete r from $R3$ and add r to $R2$.
 - (1) If $A_r P_d^k = 0$, add r to RL .
 - (2) If $A_r P_d^k < 0$, add A_r to M and update P .

52. At the conclusion of the second algorithm, the projection matrix P has the properties that $A_r P = 0$ for each $r \in R2$, $A_r P_d^k > 0$ for $r \in R3$, and $A_r P_d^k = 0$ for $r \in RL$. Numerical testing shows that the second algorithm is rarely executed.

The Karush-Kuhn-Tucker Conditions

53. The Karush-Kuhn-Tucker conditions are checked whenever $P[-\nabla f(\underline{q}^k)] = 0$. In this case the search direction is zero, and either P can be modified to give a nonzero search direction, or \underline{q}^k satisfies the Karush-Kuhn-Tucker conditions which are the necessary conditions for a minimum of f .

54. Let

$$\underline{w} = (MM^T)^{-1} M[-\nabla f(\underline{q}^k)] \quad (41)$$

where M is an $N_m \times N_p$ matrix ($N_m < N_p$) and the $\ell \times N_p$ dimensional E is assumed to occupy the first ℓ rows of M . The dimension of the column vector \underline{W} is m . (The matrix M is the same one used in the definition of the projection matrix P in Equations 34 and 40.) If the last $m - \ell$ entries in \underline{W} are less than or equal to zero and $P[-\nabla f(\underline{q}^k)] = 0$, then the Karush-Kuhn-Tucker conditions are satisfied and the procedure stops with \underline{q}^k as the optimal solution.

55. If $P[-\nabla f(\underline{q}^k)] = 0$ and one of the last $m - \ell$ components of \underline{W} is positive, one of the rows of M is removed. Specifically, if

$$W_j : \max \{W_r = r \geq \ell + 1 \text{ and } W_r > 0\} \quad (42)$$

then the j^{th} row of M is deleted and the projection matrix P is updated with this new M . The theory of Rosen (1960) guarantees then that $P[-\nabla f(\underline{q}^k)]$ is a nonzero descent direction and $M_j P[-\nabla f(\underline{q}^k)]$ is positive. Numerical experimentation indicates that this deletion of a row from M rarely occurs because of the present construction of M , thus negating the necessity of modifying P in this manner.

56. Because P has been changed, there is the possibility that $A_r P[-\nabla f(\underline{q}^k)] < 0$ for some $r \in RL$ whereupon there is a degeneracy and the routine stops. However, it is almost always the case that $A_r P[-\nabla f(\underline{q}^k)] \geq 0$ for $r \in RL$ and the line search can be initiated.

The Line Search and Stopping Criteria

57. When the line search is initiated, the nonzero descent direction is $P\underline{d}^k$, where P is a projection matrix and \underline{d}^k is either the negative gradient or Newton's direction. Furthermore, $A_r P\underline{d}^k \geq 0$ for all r for which $A_r \underline{q}^k \leq b_r$. Now define a unit vector

$$\underline{u}^k = \frac{P\underline{d}^k}{\|P\underline{d}^k\|} \quad (43)$$

and observe that P , and thus \underline{u}^k , have been constructed so that

$$E(\underline{q}^k - \lambda \underline{u}^k) = 0 \quad (44)$$

and

$$A_r(\underline{q}^k + \lambda \underline{u}^k) > 0 \quad (45)$$

for all $r \in R$. The remaining rows in A must satisfy $A_r \underline{q}^k > b_r$, but a negative value of $A_r \underline{u}^k$ will restrict the values of $\lambda \geq 0$ for which $A_r(\underline{q}^k + \lambda \underline{u}^k) \geq b_r$. Thus the maximum value of λ , λ_{\max} for which $A_r(\underline{q}^k + \lambda \underline{u}^k) \geq b_r$, or for which a violated constraint will not worsen, is defined by

$$\lambda_{\max} = \Delta_{\min} \left(\frac{b_r - A_r \underline{q}^k}{A_r \underline{u}^k} : A_r \underline{u}^k < 0, b_r - A_r \underline{q}^k < 0, r \in R \right) \quad (43)$$

If there are no indices for which $b_r - A_r \underline{q}^k < 0$ and $A_r \underline{u}^k < 0$, then λ_{\max} is set equal to a very large number, such as 10^6 .

58. The line search that is used to locate that value of λ^k for which

$$f(\underline{q}^k + \lambda^k \underline{u}^k) = \min \left\{ f(\underline{q}^k + \lambda \underline{u}^k) : 0 \leq \lambda \leq \lambda_{\max} \right\} \quad (46)$$

is Davidon's cubic interpolatory scheme described in detail by Walsh (1975). Once λ^k has been approximated, \underline{q}^{k+1} is defined to be

$$\underline{q}^{k+1} = \underline{q}^k + \lambda^k \underline{u}^k \quad (47)$$

59. The updated flow array \underline{q}^{k+1} then replaces \underline{q}^k as the solution estimate. Convergence for this procedure, and thus the solution \underline{q}^k , is established by satisfaction of the conditions presented in paragraph 36.

PART VI: SUMMARY

60. The purpose of this report was to discuss the problem of operating a multipurpose reservoir through regulation of a multilevel outlet works for a number of water quality objectives. Operation of a reservoir to meet downstream goals for multiple water quality parameters often produces conflicts; a problem formulation and solution were presented as an attempt to resolve these conflicts. The multiparameter reservoir regulation problem was formulated in terms of (a) a scalar objective function which indicates the relative value of any specified operation strategy and (b) a linear constraint set. These constraints include the hydraulic characteristics of the outlet works and any specified bounds on the release concentrations of the water quality parameters. Two different problem formulations were addressed. The target-concentration problem was formulated to achieve specific downstream target concentrations without actual constraints on the release concentrations. The constrained-concentration problem was formulated to allow the specification of upper and lower bounds for all or some of the water quality constituents. Both formulations can accurately deal with the hydraulic complexity of a multilevel outlet works.

61. The algorithms presented herein can be used in a real-time mode in which the state of the system is known by real-time measurements. The algorithms can also be used with an ecosystem simulation model in which the state of the system is predicted.

62. The algorithms provided an efficient procedure for solving the multiparameter reservoir regulation problem. The linear structure of the constraint set has been used to advantage. The problem as presented was small; most of the matrices were 3×3 , which was the dimension of the number of decision variables (open ports). The constraint matrix was larger, but calculations were done with only those constraints that were active, which was often just one or two. This solution procedure is particular to the multiparameter reservoir regulation problem; thus, the size and complexity of a general purpose nonlinear optimization code has been avoided.

63. The concept of a scalar water quality index was presented. It must be emphasized that the index was used as an example objective function for the optimization problem under consideration and that this is not a recommendation for a particular water quality index or even for the general concept of a water quality index. It was a useful tool for presenting the optimization algorithms because (a) it is a single number with functional dependence on the various parameter concentrations being considered and (b) the necessary derivatives can be determined analytically. For a particular application of the optimization procedure, a much simpler objective function might be entirely adequate and thus more appropriate.

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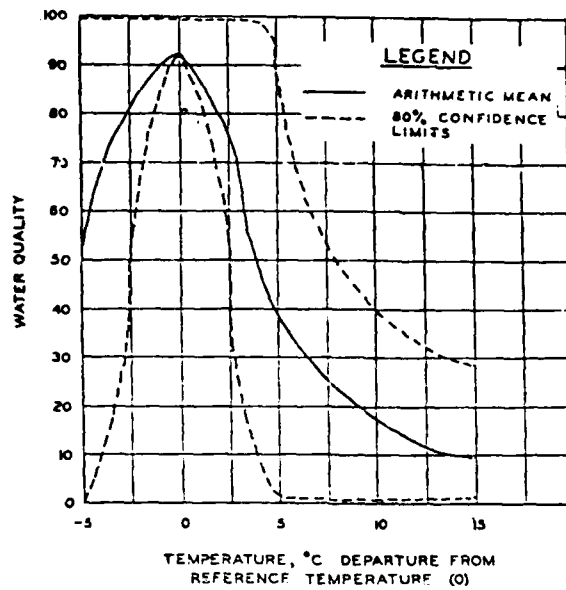
APPENDIX A: WATER QUALITY SUBINDEX FUNCTIONS
AND COEFFICIENTS (FROM KAPLAN 1974)

Table A1
Coefficients for Constrained-Concentration NSF Water Quality Subindex Polynomials

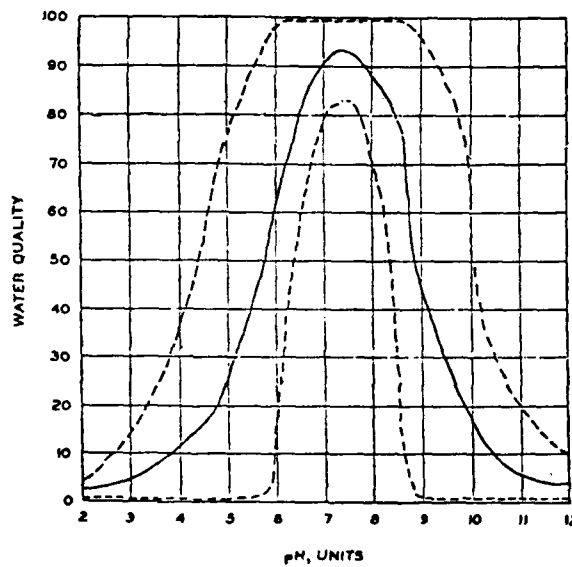
Parameters x	Polynomials: $f = a + bx + cx^2 + dx^3 + ex^4 + fx^5$					
	a	b	c	d	e	f
Temperature ($T - T_e$)	90.27	-2.564	-2.206	-0.0892	-0.0213	-0.001290
Acidity (pH)	-21.77	-42.74	17.21	-1.270		
Dissolved oxygen ($DO_{x,sat}$)	3.614	-5.140×10^{-4}	0.02412	-1.483×10^{-4}		
Total solids (TDS)	82.41	0.0947	-8.073×10^{-4}	8.477×10^{-7}		
Biochemical oxygen demand (BOD_5)	98.62	-10.628	0.4437	-6.483×10^{-3}		
Fecal coliforms (FColi)	83.37	-0.8898	5.166×10^{-3}	-1.266×10^{-5}	1.349×10^{-8}	-5.166×10^{-12}
Nitrates (NO_3)	97.06	-7.4348	0.3184	-6.266×10^{-3}	4.305×10^{-5}	
Phosphates (PO_4)	103.8	-96.27	42.59	-8.343	0.5802	

Table A2
Coefficients for Target-Concentration
Subindex Polynomials

Polynomials: $f = a + bx + cx^2$			
Where x is Release Concentration Minus Target Concentration			
Parameters x	a	b	c
Temperature (T_e)	100	0	-4.0
Acidity (pH)	100	0	-11.11
Dissolved oxygen (DO)	100	0	-4.0
Total solids (TDS)	100	0	-0.000625
Biochemical oxygen demand (BOD_5)	100	0	-0.444
Fecal coliforms (FColi)	100	0	-0.0025
Nitrogen (NO_3)	100	0	-0.16
Phosphorus (PO_4)	100	0	-16.0

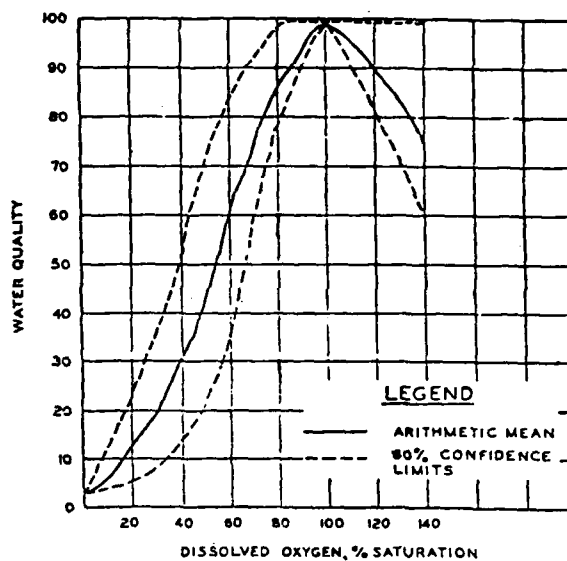


a. Temperature ($T - T_e$)



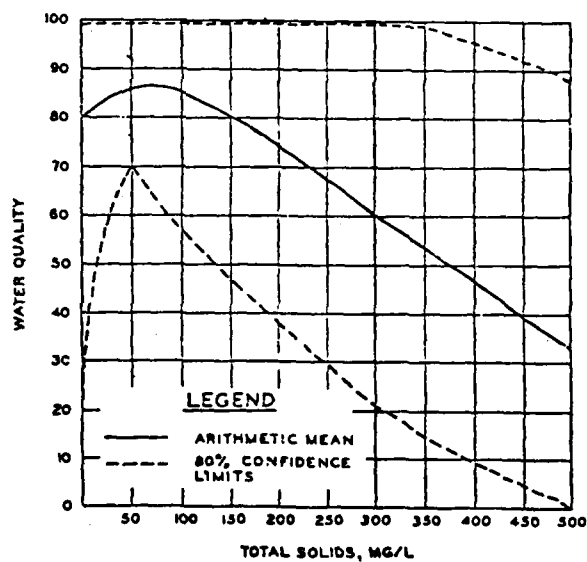
b. Acidity (pH)

Figure A1. Water quality subindices versus polynomial applications
(Kaplan 1974) (Sheet 1 of 4)



W = 0.16

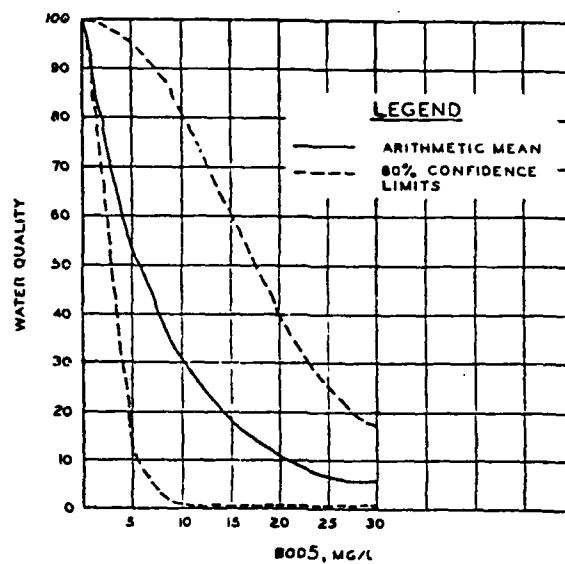
c. Dissolved oxygen ($DO_{\%sat}$)



W = 0.09

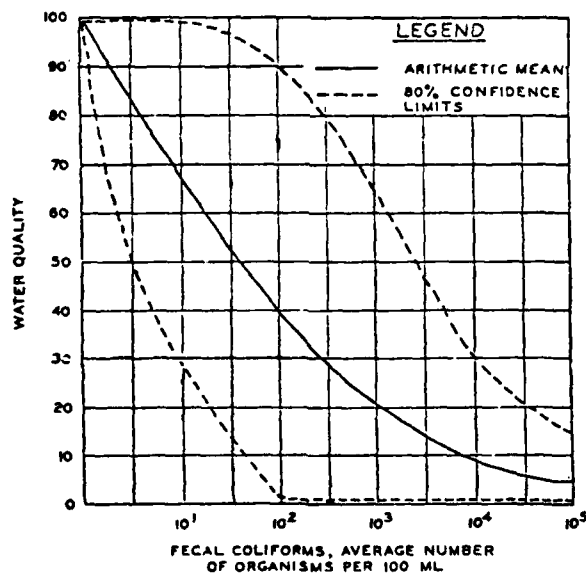
d. Total solids (TDS)

Figure A1. (Sheet 2 of 4)



W = 0.11

e. Biochemical oxygen demand (BOD₅)



W = 0.16

f. Fecal coliforms (FColi)

Figure A1. (Sheet 3 of 4)

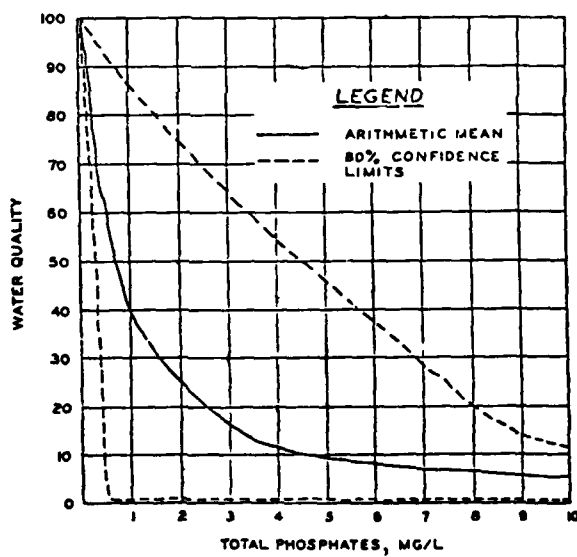
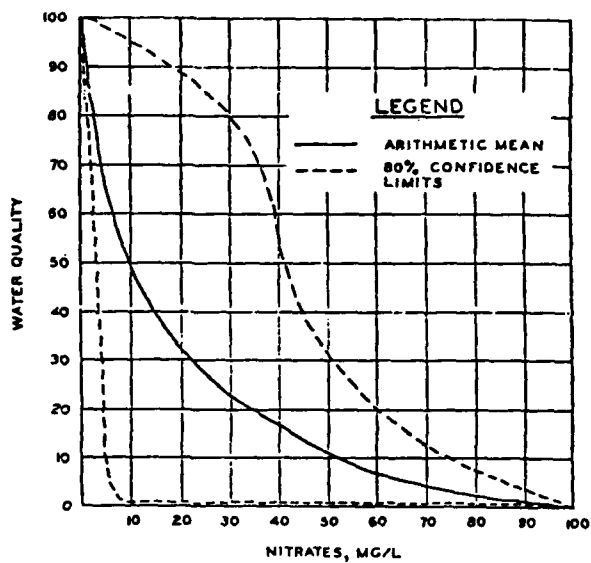


Figure A1. (Sheet 4 of 4)

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34. 7 p. : ill. ; 27 cm. -- (Technical report ; E-83-9)

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"March 1983."

Final report.

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